

WE CLAIM:

-1-

A process for producing a substituted phenol which comprises:

(a) reacting an arene with a borane selected from the group consisting of a borane with a B-H, B-B, 5 and B-Si bond in the presence of a catalytically effective amount of an iridium or rhodium complex with three or more substituents, and with or without an organic ligand selected from the group consisting of phosphorus, carbon, nitrogen, oxygen, and sulfur 10 organic ligands to produce an arylboronic ester; and

(b) oxidizing the arylboronic ester with a hydrogenating oxidizing compound to produce the substituted phenol.

-2-

The process of Claim 1 wherein the oxidizing compound is a peroxy compound selected from the group consisting of peroxymonosulfuric acid and salts thereof.

-3-

The process of Claim 1 wherein the oxidizing compound is an alkali metal peroxymonosulfate.

-4-

The process of Claim 3 wherein the alkali metal peroxymonosulfate is potassium peroxymonosulfate.

-5-

The process of Claim 1 wherein the oxidizing compound is  $2\text{KHSO}_5 \cdot \text{KHSO}_4 \cdot \text{K}_2\text{SO}_4$ .

-6-

The process of Claim 1 wherein the oxidizing compound is an organic peroxide.

-7-

The process of Claim 1 wherein the oxidizing compound is hydrogen peroxide.

-8-

The process of Claim 1 wherein the iridium complex is selected from the group consisting of  
 $(\text{Cp}^*)\text{Ir}(\text{H})_2(\text{Me}_3\text{P})$ ,  $(\text{Cp}^*)\text{Ir}(\text{H})(\text{BPin})(\text{Me}_3\text{P})$ ,  
 $(\text{Cp}^*)\text{Ir}(\text{H})(\text{C}_6\text{H}_5)(\text{Me}_3\text{P})$ ,  $(\text{Ind})\text{Ir}(\text{COD})$ ,  $(\text{Ind})\text{Ir}(\text{dppe})$ ,  
5  $(\text{MesH})\text{Ir}(\text{BPin})(\text{B}(\text{OR})_2)_2$ ,  $((\text{R}_1)_3\text{P})_3\text{Ir}(\text{B}(\text{OR}_2)_2)_3$ ,  
 $(\text{R}_1)_2\text{P})_2\text{Ir}(\text{BPin})_3$ ,  $((\text{R}_1)_2\text{P})_3\text{Ir}((\text{R}_2\text{O})_2\text{B})_3)_2$ ,  
 $((\text{R}_1)_3\text{P})_4\text{Ir}(\text{BPin})$ ,  $((\text{R}_1)_3\text{P})_2\text{Ir}(\text{BPin})_3$ ,  $(\text{MesH})\text{Ir}(\text{BPin})_3$ ,  
and  $(\text{IrCl}(\text{COD}))_2$ ,  $(\text{PMe}_3)_2\text{IrH}_5$ ,  $((\text{R}_1)_3\text{P})_2\text{IrH}_5$ , and  
 $((\text{R})_3\text{P})_2\text{IrH}_x(\text{B}(\text{OR}_2)_2)_{5-x}$  where  $x$  is 0-4, wherein  $\text{Cp}^*$  is  
10 1,2,3,4,5-pentamethylcyclopentadienyl,  $\text{BPin}$  is  
pinacolborane,  $\text{Me}$  is methyl,  $\text{H}$  is hydrogen,  $\text{P}$  is  
phosphorus,  $\text{Ind}$  is indenyl,  $\text{COD}$  is 1,5-cyclooctadiene,  
 $\text{MesH}$  is mesitylene, and wherein  $\text{R}$ ,  $\text{R}_1$ , and  $\text{R}_2$  are  
15 carbons, aryl, or a carbon in a cyclic structure.

-9-

The process of Claim 1 wherein the iridium complex is  $(\text{Ind})\text{Ir}(\text{COD})$  wherein  $\text{Ind}$  is indenyl and  $\text{COD}$  is 1,5-cyclooctadiene.

-10-

The process of Claim 1 wherein the organic ligand is a phosphorus organic ligand selected from the group consisting of trimethyl phosphine ( $\text{PMe}_3$ ), 1,2-bis(dimethylphosphino)ethane (dmpe), and 1,2-bis(diphenylphosphino)ethane (dppe).

-11-

The process of Claim 1 wherein the borane is pinacolborane (BPin).

-12-

The process of Claim 1 wherein the substituted phenol has the general formula  $\text{RR}'\text{R}''\text{Ar}(\text{OH})$  wherein R, R', and R'' are each independently selected from the group consisting of hydrogen, halo, alkyl, alkoxy, carboxylic ester, amine, and amide and wherein Ar is selected from the group consisting of aryl and heteroaryl.

-13-

A process for producing a substituted phenol which comprises:

(a) reacting in a reaction vessel an arene with a borane selected from the group consisting of a borane with a B-H, B-B, and B-Si bond in the presence of a catalytically effective amount of an iridium or rhodium complex with three or more substituents, and an organic ligand selected from the group consisting of phosphorus, carbon, nitrogen, oxygen, and sulfur organic ligands to produce an arylboronic ester; and

(b) oxidizing the arylboronic ester formed in the reaction vessel with a hydrogenating oxidizing compound to produce the substituted phenol.

-14-

The process of Claim 13 wherein the oxidizing compound is a peroxy compound selected from the group consisting of peroxymonosulfuric acid and salts thereof.

-15-

The process of Claim 13 wherein the oxidizing compound is an organic peroxide.

-16-

The process of Claim 13 wherein the oxidizing compound is hydrogen peroxide.

-17-

The process of Claim 13 wherein the oxidizing compound is an alkali metal peroxymonosulfate.

-18-

The process of Claim 15 wherein the alkali metal peroxymonosulfate is potassium peroxymonosulfate.

-19-

The process of Claim 13 wherein the oxidizing compound is  $2\text{KHSO}_5 \cdot \text{KHSO}_4 \cdot \text{K}_2\text{SO}_4$ .

-20-

The process of Claim 13 wherein the iridium complex is selected from the group consisting of

(Cp\*)Ir(H)<sub>2</sub>(Me<sub>3</sub>P), (Cp\*)Ir(H)(BPin)(Me<sub>3</sub>P),  
(Cp\*)Ir(H)(C<sub>6</sub>H<sub>5</sub>)(Me<sub>3</sub>P), (Ind)Ir(COD), (Ind)Ir(dppe),  
5 (MesH)Ir(BPin)(B(OR)<sub>2</sub>)<sub>2</sub>, ((R<sub>1</sub>)<sub>3</sub>P)<sub>3</sub>Ir(B(OR)<sub>2</sub>)<sub>2</sub>,  
(R<sub>1</sub>)<sub>2</sub>P)<sub>2</sub>Ir(BPin)<sub>3</sub>, (((R<sub>1</sub>)<sub>2</sub>P)<sub>3</sub>Ir((R<sub>2</sub>O)<sub>2</sub>B)<sub>3</sub>)<sub>2</sub>,  
((R<sub>1</sub>)<sub>3</sub>P)<sub>4</sub>Ir(BPin), ((R<sub>1</sub>)<sub>3</sub>P)<sub>2</sub>Ir(BPin)<sub>3</sub>, (MesH)Ir(BPin)<sub>3</sub>,  
and (IrCl(COD))<sub>2</sub>, (PMe<sub>3</sub>)<sub>2</sub>IrH<sub>5</sub>, ((R<sub>1</sub>)<sub>3</sub>P)<sub>2</sub>IrH<sub>5</sub>, and  
((R)<sub>3</sub>P)<sub>2</sub>IrH<sub>x</sub>(B(OR)<sub>2</sub>)<sub>5-x</sub> where x is 0-4, wherein Cp\* is  
10 1,2,3,4,5-pentamethylcyclopentadienyl, BPin is  
pinacolborane, Me is methyl, H is hydrogen, P is  
phosphorus, Ind is indenyl, COD is 1,5-cyclooctadiene,  
MesH is mesitylene, and wherein R, R<sub>1</sub>, and R<sub>2</sub> are  
15 carbons, aryl, or a carbon in a cyclic structure.

-21-

The process of Claim 13 wherein the iridium complex is (Ind)Ir(COD) wherein Ind is indenyl and COD is 1,5-cyclooctadiene.

-22-

The process of Claim 13 wherein the organic ligand is a phosphorus organic ligand selected from the group consisting of trimethyl phosphine (PMe<sub>3</sub>), 1,2-bis(dimethylphosphino)ethane (dmpe), and 1,2-  
5 bis(diphenylphosphino)ethane (dppe).

-23-

The process of Claim 13 wherein the borane is pinacolborane (BPin).

The process of Claim 13 wherein the substituted phenol has the general formula  $RR'R''Ar(OH)$  wherein R, R', and R'' are each independently selected from the group consisting of  
5 hydrogen, halo, alkyl, alkoxy, carboxylic ester, amine, and amide and wherein Ar is selected from the group consisting of aryl and heteroaryl.